Page 46 of 51 Metallomics

## **Supplementary Materials**

Evidence of Fe<sup>3+</sup> interaction with the plug domain of the outer membrane transferrin receptor protein of *Neisseria gonorrhoeae*: Implications for Fe transport

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Figure captions and figures

**Fig. SP1**: Fluorescence emission spectra of S3 peptide in the absence (band with highest intensity) and in presence of increasing aliquots of Fe(ClO<sub>4</sub>)<sub>3</sub> Conditions: 100 mM Tris at pH 7.5; [S3] = 20  $\mu$ M; with final [S3]:[Fe<sup>3+</sup>] = 1:2.5 excitation at 285 nm, using a 1 cm path length cuvette at room temperature.

**Fig. SP2**: Plots of % quenching of the 310 nm fluorescence emission band (Q%) vs total Fe<sup>3+</sup> added ([Fe]<sub>T</sub>) according to Equation (7) for **A**) peptide S2 and **B**) peptide S3 in 100 mM Tris buffer at pH 7.5. [S2] = 20  $\mu$ M; [S3] = 20  $\mu$ M. The dots represent actual data points and the smooth lines are the best fit for the data according to Equation (7) where  $K_d = 5 \times 10^{-4} \text{ M}$  for **A**) and and  $K_d = 1 \times 10^{-6} \text{ M}$  for **B**). For both S2 and S3  $Q_{max} = 100 \%$ .

Fig. SP3: Fluorescence emission spectrum of AAA mutated recombinant TbpA plug protein (EIEYE  $\rightarrow$  EIAAA), 20  $\mu$ M in 100 mM Tris at pH 7.5, excitation at 285 nm, 1 cm pathlength. The broad band at ~334 nm is attributed to excited state deprotonation of one or all of the three remaining tyrosines (Y58, Y75 and Y98). See text and ref. (1) for details.

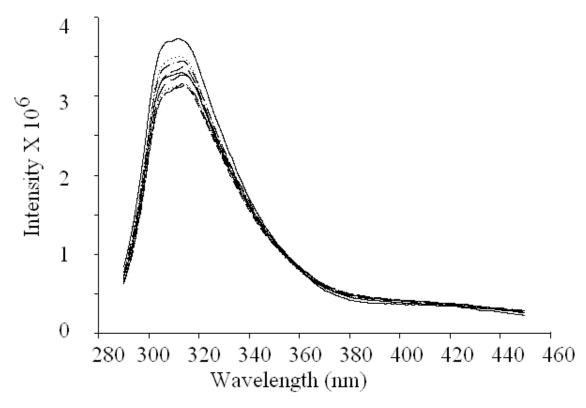
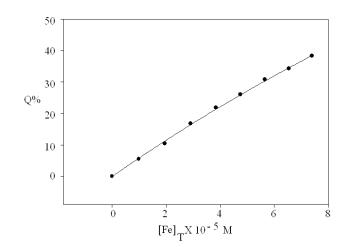
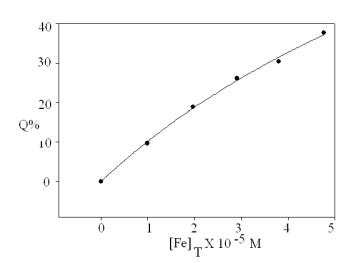


Fig. SP1





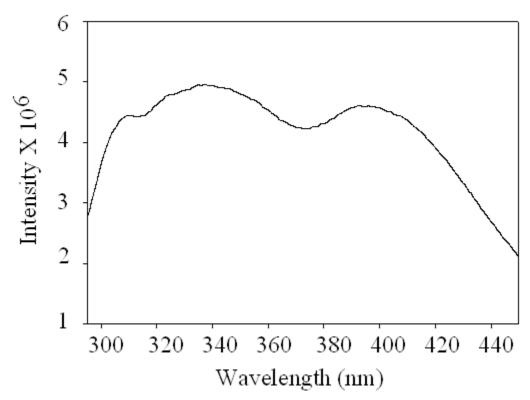


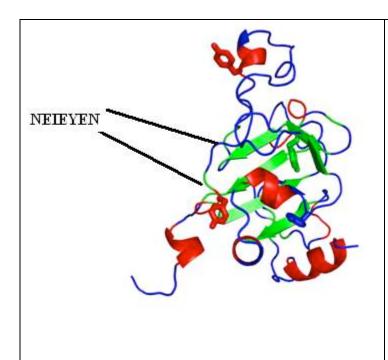
Fig. SP3

Page 50 of 51 Metallomics

## Reference

1. L. J. Libertini and E. W. Small, *Biophys. J.*, 1985, **47**, 765-772.

Metallomics Page 51 of 51



Evidence of Fe<sup>3+</sup> interaction with the plug domain of the outer membrane transferrin receptor protein of *Neisseria gonorrhoeae:* Implications for Fe transport

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A quantitative assessment is made of the ability of the TbpA plug to bind Fe<sup>3+</sup> through the sequence NEIEYEN during the transport of iron through the outer membrane to the periplasm of *Neisseria gonorrhoeae*.